AD-A260 382

UMENTATION PAGE

Form Approved OMB No 0704-0188

2. REPORT DATE 9/15/92	3. REPORT TYPE AND DATES COVERED Final 8 July 91 - 7 July 92
4. TITLE AND SUBTITLE Mathematical Analysis of Gasdynamic Wave Initiation	5. FUNDING NUMBERS DAAL03-91-G-0219
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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) University of Colorado at Boulder, Boulder, CO 80309-0026	8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) U.S. Army Research Office, P.O. Box 12211, Research Triangle Park, NC 27709-2211	10. SPONSORING/MONITORING AGENCY REPORT NUMBER ARO 28728.1-MA

DTIC ELECTE FEB 19 1993 S B D

11. SUPPLEMENTARY NOTES

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12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited.	12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

Mathematical modelling and analysis are described for studies of the dynamical response of inert or reactive systems to localized rapid power deposition. Theoretical, analytical and numerical methods are developed to find general properties of nonlinear equation systems and explicit solutions for specific initial-boundary value problems. Emphasis is placed on physical interpretation of mathematical results for the transient evolution of spatially distributed thermal and gasdynamic responses. New results are given for thermal explosion processes, for transient development of shocks and detonations, for the role of nonlinear acoustics in gascompression and for thermoacoustically induced mass transfer.

14. SUBJECT TERMS thermal explosions, reactive gasdynamics, detonations, shocks, nonlinear acoustics, perturbation methods.	15. NUMBER OF PAGES
	16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT

MATHEMATICAL ANALYSES OF GASDYNAMICS WAVE INITIATION

FINAL REPORT

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GRANT NUMBER: DAAL 03-91-G-0219

OCTOBER 6, 1992

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I. Statement of Problem

The thematic research objective of our mathematical modeling and analysis activities during the past grant period has been to develop a quantitative understanding of the dynamical response of a gaseous or solid material to localized rapid power deposition. Essential time and length scales are obtained from a study of nondimensionalized equation systems. Perturbation methods are used to reduce complex mathematical systems to more elementary forms, valid in some specifically defined limit. Then analysis and numerical methods are used to find basic general properties of the equation systems and solutions for specific boundary and initial conditions. The transient evolution of thermal and gasdynamical responses to internal and external power deposition and mechanical disturbances is considered for both inert and reactive systems. The summary of activities to follow describes published, submitted and "in-preparation" papers in each of several research areas, and includes a brief comment about the objectives of the studies and the methods employed.

II. Summary of Results and Publication List

A. Shock Wave Initiation and Evolution

A boundary power deposition disturbance is used to create shock waves in an inert gas. An initial-boundary value analysis is used for a planar system. Perturbation methods are used to find crucial time and length scales that are of importance in each of several physical regimes. Analytical and numerical methods are used to find solutions that describe transient shock wave and subsequent flow field evolution. Results are given for both constant and time-dependent boundary heating.

1. A. A. Sileem and D. R. Kassoy, "Shock Wave Generation and Propagation in Gases Due to Boundary Power Deposition," revision in progress (1992).

Abstract. The initiation, and subsequent propagation of a planar unsteady shock wave in an inert gas confined between two parallel plane walls is considered, when there is time-dependent power deposition at the boundary. A numerical solution is obtained for the Euler equations that describe the flow driven by the moving edge of an expanding conduction layer as formulated in earlier work by Kassoy and co-workers. The solution is obtained by using the explicit, finite-difference MacCormack scheme with the Flux-Corrected Transport technique to reduce the oscillations wherever large gradients exist.

The results show that the numerical code is capable of capturing shock waves with excellent accuracy. The pressure and velocity at the edge of the conduction layer increase as the

power deposition at the boundary increases with time. Accordingly, the shock speed and strength increase with time. The increase in the pressure level with time provides a source of compression heating in the gas contained in the conduction layer. The spatially variable fluid properties between the edge of the conduction layer and the shock are found for several different time-dependent functions of the power deposition at the boundary.

B. Detonation Initiation and Evolution

This study is focused on the birth and evolution of planar detonations arising from purely thermal disturbances in a reactive gas. An initial-boundary value problem approach has been used where the initiating disturbance is provided by volumetric internal heating. An Euler code based on the MacCormack method is employed to find explicit solutions. Numerical data has been evaluated to demonstrate the propagation of gasdynamic and reactive waves, the appearance of localized thermal explosions and the formation of ZND-type detonations.

1. A. A. Sileem, D. R. Kassoy and A. R. Hayashi, "Thermally Initiated Detonation Through Deflagration to Detonation Transition," Proc. Roy. Soc. Lond. A **435**, (1991), 459–482.

   Abstract. The initiation of a planar detonation via deflagration to detonation transition (DDT) is studied in a reactive mixture confined between two infinite parallel plane walls. The mixture is ignited by bulk power deposition of limited duration in a thin layer adjacent to the left-hand wall. A combustion wave starts to propagate into the reactant, supported by expansion of the burned hot gases. Compression waves generated ahead of the combustion front coalesce quickly to form a shock wave strong enough to trigger considerable chemical reaction. This newly started reaction evolves into a reaction center in which the chemical heat release rate increases rapidly. The subsequent explosion of the reaction center creates compression waves that steepen to form a new shock. The strengthened lead shock ignites a new strongly coupled reaction zone that supports the formation of an initially overdriven detonation. Subsequently, the wave decays to an oscillating planar detonation with mean properties of a C. J. wave.

2. J. Kuehn and D. R. Kassoy, "Further Results on Thermally Initiated Detonations," work in progress (1992).

   Abstract. Extensive, detailed evaluation of the numerical method used in Sileem, Kassoy and Hayashi (1991) [see item 1 above] is used to show that the longtime solution for the thermally initiated detonation asymptotes without oscillations to the C.J. wave state.

The fully transient development processes prior to the appearance of a decaying overdriven wave are verified. Solution properties for a range of bulk power deposition, heat of reaction and activation energy parameters are described. Unfortunately, the numerical method cannot be used in parameter ranges where pulsating or oscillating detonations are predicted in piston-supported systems.

C. Steady State High Speed Reaction Zone Structure

This research effort is focused on describing the flow, thermal and chemical structure in the reaction zone behind a steady state normal shock. A major goal is to predict the length scales for the reactive processes, given specific chemical kinetic steps. Perturbation methods, developed originally in ARO-supported research on classical thermal explosion theory, are used to develop solutions for this compressible flow problem.

1. K. Kirkkopru and D. R. Kassoy, "Dissociation–Recombination Relaxation Behind a Normal Shock," Phys. Fluids A **3**, (1991), 2777–2785.

   Abstract. Mathematical methods developed originally for thermal explosion theory are used to study the evolution of a dissociation–recombination process occurring in a compressible gas behind a normal shock. The dissociation–recombination reaction, $AB + M \rightleftharpoons A + B + M$, is assumed to have a relatively large dissociation temperature, so that high activation energy perturbation techniques can be used to derive general parameter dependent *analytical* solutions. Spatial variation of the dependent variables is described in three zones, each of distinct length scale and physical character. Initially, small changes in temperature, concentrations, density and pressure occur in the relatively high temperature dissociation initiation zone. In the subsequent broader major dissociation region, most of the specie AB is converted to A and B and there are significant variations in all physical variables. In the last and thickest zone, recombination becomes important as the reactive flow evolves to a final equilibrium state. The results provide an analytical counterpart to numerical solutions obtained earlier for the now classical problem of idealized diatomic gas dissociation.

D. Mass Transport Due to Internal Power Deposition

The objective of this work is to predict quantitatively the mass transport induced when spatially distributed, transient power deposition occurs in a confined inert gas. Perturbation methods and asymptotic expansions, valid for the low Mach number (of the induced gas velocity) limit, are used to develop solutions.

1. Sutrisno and D. R. Kassoy, "The Interaction of Thermoacoustic and Natural Convection in a Confined Gas Subjected to Boundary Heating," submitted, J. Eng. Math (1991), revision in progress (1992).

   Abstract. Thermal power deposition through the vertical surfaces of a rectangular container enclosing gaseous helium initiates fluid motion through thermoacoustic and buoyancy effects. When the surface temperature rise on the acoustic timescale of the container is comparable with the initial value, conduction heating takes place only in a thin, continuously growing boundary layer near the heated wall. The horizontal expansion of the hot gas produces a piston-like effect at the boundary layer edge. The edge of the expanding conduction layer induces compressive acoustic disturbances in the essentially isentropic core region. Repeated passage of the acoustic disturbances across the core produces constantly increasing, accumulated temperature, pressure and density disturbances. A vertically aligned downward gravity field creates buoyancy forces in the hot conductive boundary layers that cause upward natural convection of the heated fluid. On the other hand, the fluid motion in the unheated, and acoustically compressed core, is downward, the result of a balance between weak buoyant forces, and an induced vertical pressure gradient. A systematic analysis using various perturbation techniques is carried out to obtain solutions in both the boundary layer and the core. The theory is based on a complete system of conservation equations governing viscous, heat conducting and compressible flow.

2. A. Herczynski and D. R. Kassoy, "Response of a Confined Gas to Volumetric Heating in the Absence of Gravity II: Fast Transients," in preparation (1992).

   Abstract. A one-dimensional model of the motion induced by a rapidly varying volumetric heat source in a confined gas at zero-gravity is constructed. The model complements the slow-transients theory developed by the authors previously and is applicable to processes involving exothermic reactions or radiation heating of a gas occurring on acoustic time-scale in weightlessness. The response of a compressible fluid to transient bulk heating is analyzed by means of asymptotic methods. It is found, that modulating heating causes gas to oscillate in the container. The initial rest state of a fluid determines the set of resonant frequencies, at which the amplitude of the induced flow grows rapidly. If the fast-transient heating persists on a long time-scale, the basic thermodynamic state of a gas is altered and the resonant frequencies shift. Superimposed on this long time evolution are continuing acoustic disturbances propagating in the medium.

E. Thermal Explosion Phenomena

The object of this study is to give a precise, accurate description of the ignition process for reactive–diffusive and reactive-Euler induction period models. For reactive–diffusive self-ignition processes, we can now mathematically describe the progress of self-ignition right up to the time when combustion ceases in the core of the hot spot, very little hindered by diffusive losses.

1. J. Bebernes and A. Lacy, Finite time blowup for reactive–diffusive systems, J. Differential Equations, **95** (1991), 105–129.

Abstract. This paper deals with initial-boundary value problems for parabolic systems of the form

$$(1.1) \qquad \begin{cases} \begin{matrix} u_t - \Delta u = (1-v)f(u) \\ v_t - \Delta v = (1-v)f(u) \end{matrix}, & x \in \Omega \subset \mathbb{R}^n, \quad t > 0 \\ u(x,0) = u_0(x) \geq 0, \quad 0 \leq v(x,0) = v_0(x) \leq 1, & x \in \Omega \\ \dfrac{\partial u}{\partial n} + \mu u = 0, \quad \dfrac{\partial v}{\partial n} + \nu v = 0, \quad \mu, \nu \in [0,\infty] & x \in \partial\Omega, \quad t > 0, \end{cases}$$

where $\Omega \subset \mathbb{R}^n$ is a bounded domain with smooth boundary $\partial\Omega$, $u_0(x)$ and $v_0(x)$ are continuous, bounded, nonnegative functions, and $f(s)$ is assumed to be C^2 with $f(s) > 0$, $f'(s) > 0$, $f''(s) > 0$, and $f(s) \gg s^2$ for $s \to \infty$. Additional assumptions will be imposed as needed in the next three sections.

Problem (1.1) arises as an approximating model for an exothermic chemical reaction taking place within a porous medium assuming one diffusing reactant and the Frank–Kamenetski approximation $f(u) = e^u$ for the classical Arrhenius rate law. In this case u and v are chosen to that physically the scaled temperature of the reaction process above ambient is u and the scaled concentration is $1 - v$.

Problem (1.1) ([1], [2]) has a unique nonnegative classical solution on $\pi_\sigma = \Omega \times [0, \sigma)$. By this, we mean a pair of nonnegative $C^{2,1}$ functions $(u(x,t),\ v(x,t))$ which satisfy (1.1) in π_σ. For a given solution (u, v) of (1.1), define

$$(1.2) \qquad T = \sup\left\{\sigma > 0 : (u,v) \text{ is a bounded solution of (1.1) on } \pi_\sigma\right\}$$

The purpose of this paper is to determine in terms of u_0, v_0, μ, ν, f and Ω the cases $T = +\infty$ and $T < +\infty$. If $T = +\infty$, the solution exists for all time $t > 0$ and is global. If

$T < +\infty$, then

$$\limsup_{t \to T} \left[\|u(t)\|_\infty + \|v(t)\|_\infty \right] = +\infty \tag{1.3}$$

since otherwise the solution could be extended beyond T. When (1.3) holds, with $T < \infty$, we say that the solution *blows up in finite time.*

2. J. Bebernes and S. Bricher, Final time blowup profiles for semilinear parabolic equations via center manifold theory, SIAM J. Math. Anal. **23** (1992), 852–869.

Abstract. In this paper we consider the semilinear parabolic equation $u_t = \Delta u + f(u)$ in $\mathbb{R}^n \times (0, \infty)$ where $f(u) = e^u$ or $f(u) = u^p$, $p > 1$. For any initial data that is a positive, radially decreasing lower solution, and that causes the corresponding solution $u(x,t)$ to blow up at $(0,T) \in \mathbb{R}^n \times (0,\infty)$, we prove by using techniques from center manifold theory that the final time blowup profiles satisfy:

$$u(x,T) = -2\ln|x| + \ln|\ln|x|| + \ln 8 + o(1) \qquad \text{for } f(u) = e^u,$$
$$u(x,T) = \left(\frac{8\beta^2 p|\ln|x||}{|x|^2}\right)^\beta (1 + o(1)) \qquad \text{for } f(u) = u^p$$

as $|x| \to 0$.

3. J. Bebernes, S. Bricher, and V. Galaktionov, Asymptotics of blowup for weakly quasilinear parabolic problems, Journal of Nonlinear Analysis, in press (1992).

Abstract. The blowup asymptotics of classical solutions $u = u(|x|, t)$ of the Cauchy problem and the initial-boundary value problem for the weakly quasilinear heat equation

$$u_t = \nabla \cdot (k(u)\nabla u) + Q(u)$$

and analyzed, assuming that $k(u) = 1 + p(u)$, $Q(u) = e^u(1 + q(u))$ with $p, q \to 0$ as $u \to \infty$ and small along with their first two derivatives. We prove that many asymptotic properties for the semilinear equation $u_t = \Delta u + e^u$ remain valid after weak quasilinear perturbations of the elliptic operator.

III. Participants

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IV. Report of Inventions

None.